Hydrodynamics of thermal granular convection

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A hydrodynamic theory is formulated for buoyancy-driven ("thermal") granular convection, recently predicted in molecular dynamic simulations and observed in experiment. The limit of a dilute flow is considered. The problem is fully described by three scaled parameters. The convection occurs via a supercritical bifurcation, the inelasticity of the collisions being the control parameter. The theory is expected to be valid for small Knudsen numbers and nearly elastic grain collisions.

As we know from experience, hot fluid rises. Is the same statement true for *granular* fluid, where the role of temperature is played by fluctuations of the grain velocities? There is strong recent evidence that the answer to this question is positive. Buoyancy-driven "thermal" granular convection was first observed in molecular dynamic (MD) simulations of granular gas in two dimensions [1], with no shear or time-dependence introduced by the system boundaries. It was found that thermal granular convection appears via a supercritical bifurcation, with inelastic collision losses being the control parameter [1]. Strong evidence for thermal granular convection was recently obtained in experiment with a highly fluidized 3D granular flow [2] (see also an earlier work [3]). In these two systems [1,2] the convection is driven by a negative vertical granular temperature gradient [4] which makes this convection similar to the classical Rayleigh-Bènard convection [5] and its analogs in compressible fluid [6–9]. In the Rayleigh-Bènard problem a negative temperature gradient is imposed externally. In a granular flow driven from below, it develops spontaneously because of the inelasticity of particle collisions [10].

The phenomenon of "thermal" convection in granular fluids is fascinating, as it gives one more example of similarities/differences between the granular and "classical" fluids [11]. Though basic properties of thermal granular convection were investigated in the MD simulations [1], no theory exists yet. The objective of the present work is to formulate such a theory. We will work in the regime where the "standard" granular hydrodynamic equations in 2D [12], systematically derivable from kinetic equations [13], are expected to be accurate. As it has become clear by now [13], this requires (in addition to the strong inequality $K \ll 1$, see below, and sufficiently low density) that particle collisions be nearly elastic: $q \ll 1$, where $q = (1 - r)/2$ is the inelasticity coefficient and r is the normal restitution coefficient. The nearly elastic limit is motivated by the MD simulations [1] where convection was observed already at very small inelasticities: $4 \times 10^{-4} \le q \le 2 \times 10^{-2}$. As in the MD simulations [1], we will assume a velocity-independent restitution coefficient.

We will limit ourselves to dilute flow, $n \ll n_c$, where n is the number density of the grains and n_c is the close-packing density. As thermal granular convection does not necessarily involve clustering, the latter assumption is not too restricting.

Here is an outline of the rest of this Communication. We will see that the hydrodynamic problem of thermal granular convection is fully determined by *three* scaled parameters: the Froude number F, Knudsen number $K \ll 1$ and inelasticity coefficient $q \ll 1$, and by the aspect ratio of the system. The translationally symmetric static steady state of the system plays the role of the "simple conducting state" of the Rayleigh-Bènard problem. By employing the Lagrangian mass coordinate, we find this steady state analytically. Then, by solving the granular hydrodynamic equations in a square box by a Lattice-Boltzmann method, we observe a supercritical bifurcation at a critical value of $q = q_c$ and steady convection at $q > q_c$, in qualitative agreement with MD simulations [1] and experiment [2]. We then investigate the dependence of the convection threshold q_c on K and F. Our results open the way to a systematic investigation of thermal granular convection.

Let $N \gg 1$ identical smooth hard disks with diameter d and mass m move without friction and inelastically collide inside a two-dimensional box with lateral dimension L_x and height L_y. The aspect ratio of the system $\Delta = L_x / L_y$. The gravity acceleration g is in the negative y direction. The particles are driven by a base that is kept at temperature T_0. For simplicity, the three other walls are assumed elastic. The hydrodynamic description deals with coarse-grained fields: the number density of grains $n(\mathbf{r}, t)$, granular temperature $T(\mathbf{r}, t)$ and mean velocity of grains $\mathbf{v}(\mathbf{r}, t)$. The governing equations can be written, in the dilute limit, in the following scaled form:

$$\frac{dn}{dt} + n \, \nabla \cdot \mathbf{v} = 0 \,, \tag{1}$$

$$n \, d\mathbf{v}/dt = \nabla \cdot \mathbf{P} - F \, n \, \mathbf{e_y} \tag{2}$$

$$n \, dT/dt + nT \, \nabla \cdot \mathbf{v} =$$

$$K \left[\nabla \cdot (T^{1/2} \nabla T) - R\, n^2\, T^{3/2} \right] . \qquad (3)$$

Here $\mathbf{e_y}$ is the unit vector along y, d/dt is the total derivative, $\mathbf{P} = -nT\,\mathbf{I} + \frac{1}{2}\,K\,T^{1/2}\,\hat{\mathbf{D}}$ is the stress tensor, $\mathbf{D} = (1/2)\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^T\right)$ is the rate of deformation tensor, $\hat{\mathbf{D}} = \mathbf{D} - (1/2)\,tr\,(\mathbf{D})\,\mathbf{I}$ is the deviatoric part of $\mathbf{D}$ and $\mathbf{I}$ is the identity tensor. In the dilute limit the bulk viscosity can be neglected compared to the shear viscosity [12]. In addition, we neglected the small viscous heating term in the heat balance equation (3). The three scaled parameters entering Eqs. (2) and (3) are the Froude number $F = mgL_y/T_0$, the Knudsen number $K = 2\pi^{-1/2}\,(d\,L_y\,\langle n\rangle)^{-1}$, and the collision losses parameter $R = 8q\,K^{-2}$. R will be used through the rest of this Communication instead of the inelasticity coefficient q. The Knudsen number K is of order of the ratio of the mean free path of the grains to the system height. For hydrodynamics to be valid we should demand $K \ll 1$. The units of distance, time, velocity, density and temperature in the scaled equations are L_y, $L_y/T_0^{1/2}$, $T_0^{1/2}$, $\langle n\rangle$ and T_0, respectively. Finally, $\langle n\rangle = N/(L_x L_y)$ is the average number density of the grains.

The physical meaning of the scaled numbers F, K and R is clear. The Froude number F determines the relative role of the maximum potential energy of grains in the gravity field and their maximum fluctuation energy supplied by the driving base. The Knudsen number K determines the efficiency of the momentum and energy transport in the system. In the hard-sphere fluid we are working with, the kinematic viscosity and thermal diffusivity are equal to each other, so the Prandtl number is equal to 1. The inelastic heat loss number R determines the relative role of the inelastic heat losses and heat conduction.

The boundary conditions are $T(x, y=0, t) = 1$ with a zero heat flux at the rest of the boundaries. Also, we demand zero normal components of the velocity and slip (no-stress) conditions at all boundaries. The total number of particles is conserved:

$$\frac{1}{\Delta} \int_0^\Delta dx \int_0^1 dy\, n(x, y, t) = 1 . \qquad (4)$$

Therefore, in the hydrodynamic formulation, the problem is characterized by F, K and R and the aspect ratio Δ, instead of the full set of 8 parameters $m, d, q, L_x, L_y, g, T_0$ and N.

Translationally symmetric static steady states are described by the one-dimensional equations considered in many works (see, e.g. Ref. [14]):

$$(n_s T_s)' + F\, n_s = 0 \qquad (5)$$

and

$$(T_s^{1/2} T_s')' - R\, n_s^2 T_s^{3/2} = 0 \qquad (6)$$

(primes denote y-derivatives). In our problem these equations are complemented by the boundary conditions $T_s(y=0) = 1$ and $T_s'(y=1) = 0$ and normalization condition $\int_0^1 dy\, n_s(y) = 1$. A static state is characterized by the scaled numbers F and R. Equations (5) and (6) can be solved by going over to the Lagrangian mass coordinate $\mu(y) = \int_0^y n_s(y')\, dy'$ [15]. In view of Eq. (4), the Lagrangian mass coordinate μ changes between 0 and 1. First, we solve Eq. (5) for $n_s(\mu)$:

$$n_s(\mu) = \frac{p_0 - F\,\mu}{T_s(\mu)} , \qquad (7)$$

where p_0 is the (as yet unknown) pressure at the thermal base $\mu = 0$. Substituting this relation into Eq. (6), we obtain a *linear* equation for $Y(\mu) \equiv T_s^{1/2}(\mu)$:

$$(\lambda - \mu)\,Y'' - Y' - (R/2)\,(\lambda - \mu)\,Y = 0 , \qquad (8)$$

where $\lambda = p_0/F$ and the primes now stand for μ-derivatives. The general solution of Eq. (8) is a linear combination of the Bessel functions $I_0[\sqrt{R/2}(\lambda - \mu)]$ and $K_0[\sqrt{R/2}(\lambda - \mu)]$. The two arbitrary constants are found from the boundary conditions $Y(\mu = 0) = 1$ and $Y'(\mu = 1) = 0$. Now we employ Eq. (7) for $n_s(\mu)$ and determine the Eulerian coordinate $y = y(\mu)$ by calculating $y = \int_0^\mu d\mu'/n_s(\mu')$. Demanding that $y(\mu = 1) = 1$, we find λ (and, therefore, p_0) which completes the solution. An example of static temperature and density profiles is shown in Fig. 1. We found that, at $F = 0.1$ and $R \lesssim 0.7$, the temperature difference between the lower and upper plates in the static solution agrees very well with the MD simulations results [1]. The negative temperature gradient is clearly seen in Fig. 1. At sufficiently large R, a denser and heavier gas is located on top of the underdense gas. This destabilizing factor drives convection. The stabilizing factors are granular viscosity and heat conduction.

We investigated convective (in)stability of the static state by solving the time-dependent hydrodynamic equations (1)-(3) numerically. A lattice-Boltzmann scheme, previously used to study the classical Rayleigh-Bènard convection [16], was employed. The scheme give accurate results for moderate density variations which was the case in the parameter range of this study. Like in the MD simulations [1], we considered a square box: $\Delta = 1$. The initial conditions were the following: a uniform (and equal to 1) temperature, zero velocity and density equal to 1 plus a small sinusoidal perturbation. We fixed F and K and varied R. The presence (absence) of convection in the box was measured by computing (after transients die out) the velocity circulation $C = \oint \mathbf{v} \cdot \mathbf{dl}$ along the edges of the box. In all cases a zero circulation is observed at sufficiently small R, and the flow approaches a static steady state. We checked that the density and temperature profiles of the steady state, obtained in the

lattice-Boltzmann simulations, agree within 1.5 % with the analytic solutions of Eqs. (5) and (6). Convection always develops, via a supercritical bifurcation, when R exceeds a critical value $R_c(F, K)$. Figure 2 shows steady convection that appears in this system after transients decay. Figure 3 shows the bifurcation diagram. The same type of bifurcation (supercritical bifurcation) was observed in the MD simulations [1].
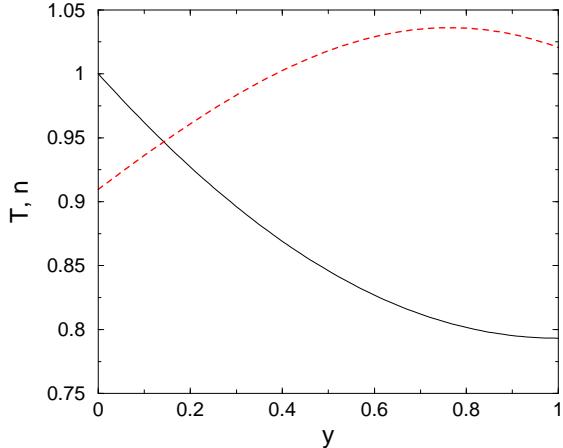

FIG. 1. One-dimensional static temperature (solid line) and density (dashed line) profiles for $F = 0.1$ and $R = 0.5$.
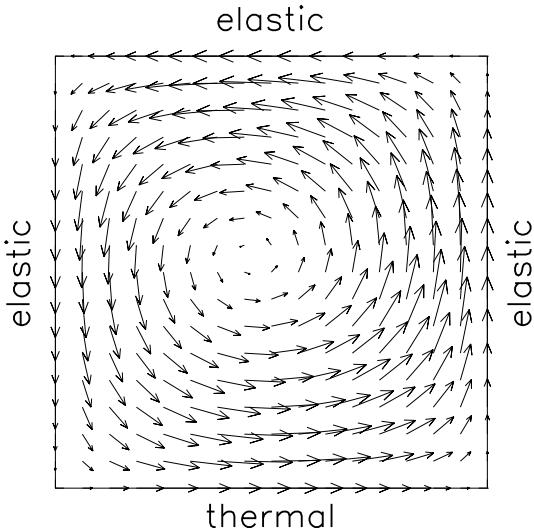
FIG. 2. Steady-state hydrodynamic velocity field for $F = 0.1$, $K = 0.02$ and $R = 3.6$.

We determined the convection onsets and bifurcation diagrams for two values of the Froude number: $F = 0.05$ and 0.1, varying the Knudsen number K between 0.01 and 0.06. The results of this series of simulations, depicted in Fig. 4, clearly show that the viscosity and heat conduction (both of which scale like K) are stabilizing factors. Also, it can be seen that stronger gravity promotes convection as expected.
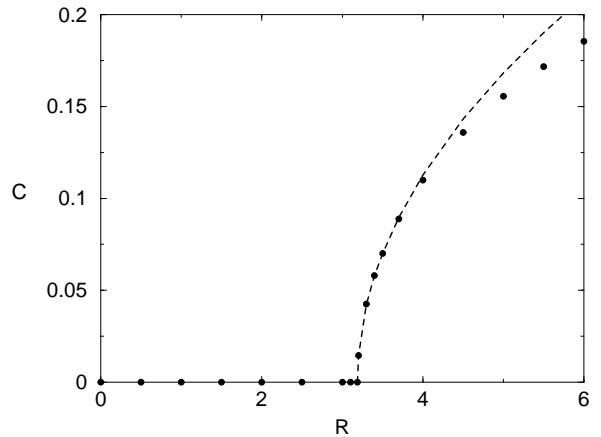

FIG. 3. Velocity circulation C along the edge of the box vs. R measured in hydrodynamic simulations (points), and the curve $0.125\,(R - 3.186)^{1/2}$ (dashed line). In this example $F = 0.1$ and $K = 0.05$.
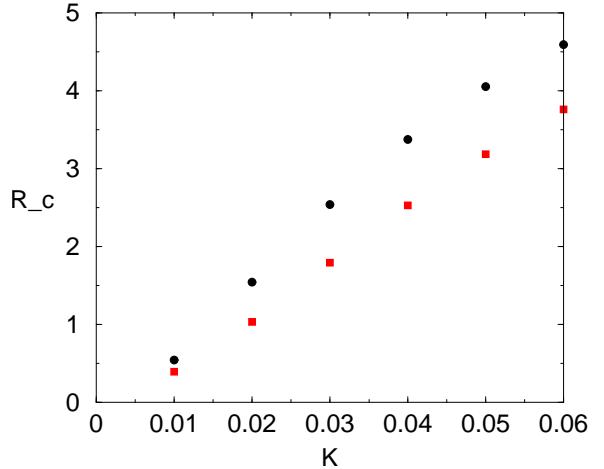

FIG. 4. The critical value R_c for the convection onset vs. the Knudsen number K for $F = 0.05$ (circles) and 0.1 (squares).

Transient motions in the system were investigated by monitoring the maximum value of the hydrodynamic velocity in the system as a function of time. After initial transients decay, the dynamics depends on whether one is in the subcritical ($R < R_c$) or supercritical ($R > R_c$) range. We found that, in the supercritical range, the maximum velocity first increases exponentially in time (no "overstability"), and then approaches, in an oscillatory way, a constant value corresponding to a steady convection. We used the growth rates to extrapolate to the critical values R_c for the convection onset. We also found that the frequency of the decaying oscillations around the steady convection vanishes at the convection onset.

The next theoretical step should be the linear stability analysis of Eqs. (1)-(3) around the static solutions, and a detailed investigation of the hydrodynamic modes of the system. In the spirit of pattern formation theory [17],

one should also study convection in a strip infinite in the lateral direction, by varying the lateral wave number of the perturbation. This analysis is presently under way.

Observing thermal granular convection in experiment requires several conditions, some of which can be stringent. A detailed discussion of these conditions is beyond the scope of this Communication. However, there is one crucial issue that has to be discussed. A standard method of fluidization of granular materials (used, in particular, in experiment [2]) is vibration of the bottom plate. There are two important *necessary* conditions for observing thermal granular convection in vibrofluidized granular beds. Firstly, the frequency of vibration of the bottom plate should be much higher than any relevant *macroscopic* frequency of the granulate (like the frequency of the bed oscillations or inverse sound travel time). Secondly, the vibration amplitude should be less than the mean free path of the granulate near the bottom wall. These conditions guarantee that there is no direct coupling between the bottom plate vibration and collective granular motion. Additional conditions are those of convection instability. Our theory gives such a condition: $R > R_c(K, F)$. However, we obtained this condition (a) in the dilute limit $n \ll n_c$, and (b) for a "thermal", rather than vibrating, bottom plate. Limitation (a) can be severe unless the experiment is done in a 2D geometry (spherical particles rolling on a slightly inclined smooth surface and driven by a vibrating wall [18]). To what extent is limitation (b) severe? A full quantitative answer to this question requires solving a similar hydrodynamic problem, but with a different boundary condition [14,19] that mimics the vibrating wall more directly. Based on an analogy with other driven granular systems [20], we expect that the results obtained for the two boundary conditions will not differ too much from each other, at least qualitatively.

Finally, it is possible that the concept of "thermal" convection can be applicable to some granular systems driven by shear. A recent example is the longitudinal vortices observed in experiment on rapid granular flow in a chute [21].

To summarize, granular hydrodynamics provide a proper language for the problem of thermal granular convection and open the way to a systematic investigation of this and related phenomena.

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